Ground state of antiferromagnetic Heisenberg two-leg ladder in terms of the valence-bond solid picture

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Abstract

We have proposed the plaquette-singlet solid (PSS) ground state for the spin-1 antiferromagnetic Heisenberg twoleg ladder. Based on the PSS picture, we discuss the correspondence of the PSS state to the valence-bond solid (VBS) state of the ground state of spin-2 chain by introducing an appropriate composite spin picture. When the bond alternation is introduced, there occur quantum phase transitions and each phase can be identified with that in the dimerized spin-2 chain. Furthermore, we argue that the VBS picture of spin-2S chain can be applied to the ground state of spin-S two-leg ladder.

Key words: quantum spin ladder; valence-bond solid picture; plaquette-singlet solid picture; quantum Monte Carlo method

Ground state of one-dimensional quantum spin systems in general has no long-range order due to strong quantum fluctuations. A typical example investigated so far is the celebrated Haldane gap system. The well-established valence-bond solid (VBS) picture [1] gives the intuitive understanding for the ground state of such spin chains. Especially for the spin-1 antiferromagnetic (AF) Heisenberg chain the hidden AF order [2] in the ground state has been discussed. This is an interesting argument that shows a disordered state realized by quantum fluctuations is not totally disordered, but has some kind of topological hidden order.

In Ref. [3], we have discussed the ground state and its hidden order of the spin-1 AF Heisenberg two-leg ladder, in which the naive VBS picture breaks down. The spin-1 ladder has a gapped ground state irrespective of the ratio between the strength of the rung coupling and the leg coupling, including the two limits of independent rung dimers and two decoupled spin-1 Haldane chains. In the VBS picture for these two limiting cases, the valence bonds are located on the rungs and legs, respectively. Thus the states characterized by the different valence-bond configurations are in the same phase. We focused on a singlet wavefunction of the four S=1/2 spins on the plaquette between the two nearest rungs. It can be written as a linear combination of the rung valence bonds and the leg valence bonds. We have shown that the ground state of the spin-1 two-leg ladder is described well by the wave function constructed from the spin-1/2 plaquette singlets [3]. This is called the plaquette-singlet solid (PSS) picture.

It is interesting to see that there is no quantum phase transition in the spin-1 AF ladder with the in-phase bond alternation [3,4], while it exhibits quantum phase transitions in the presence of the anti-phase bond alternation [5,6]. What does this difference with respect to the bond alternation pattern suggest? Furthermore, the spin-1 ladder with the ferromagnetic rung coupling

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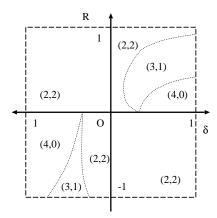


Fig. 1. Schematic ground-state phase diagram of the spin-1 ladder. The parameters R and δ denote the strength of rung coupling and the dimerization, respectively. The right (left) half shows the anti-phase (in-phase) bond-alternation case. There exist quantum critical lines only in the upper-right and down-left regions. Each phase in the phase diagram can be identified with the VBS state for the composite S=2 diagonal (rung) spin for R>0 (R<0).

is equivalent to the spin-2 chain in the strong coupling limit, which exhibits quantum phase transitions between (2,2)-, (3,1)-, and (4,0)-phases in the presence of bond alternation, where the indices (m,n) denotes the valence-bond configuration with m (n) valence bonds on odd (even) bonds [7]. What about the spin-1 ladder with the weak ferromagnetic rung coupling and bond alternation? In the following we will discuss these questions in detail.

The Hamiltonian for the spin-1 two-leg ladder is given by

$$H = \sum_{i=1,2} \sum_{j} J_{i,j} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} + K \sum_{j} \mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j}, \quad (1)$$

where $\mathbf{S}_{i,j}$ denotes the jth spin on the ith leg. We consider the cases with in-phase bond alternation $J_{i,j} = J[1 + (-1)^j \delta]$ and with anti-phase bond alternation $J_{i,j} = J[1 + (-1)^{i+j} \delta]$. The schematic ground-state phase diagram, parametrized by the strength of bond alternation δ and the rung coupling R = K/(J+|K|), is shown in Fig. 1. The phase boundaries are determined precisely by the quantum Monte Carlo method [8].

In the AF rung region (R>0) with anti-phase dimerization (right-upper in Fig. 1), there are three different phases. They can be identified as the (2,2)-, (3,1)-, and (4,0)-VBS states for the spin-2 dimerized chain, respectively. This is done by making S=2 composite spins from the two S=1 spins situated at the diagonal position in a plaquette between the nearest neighbor rungs. For example, in the PSS state, where two parallel valence bonds locate on either the rung edges or the leg edges of a plaquette, diagonal composite spins always have two valence bonds in-between.

Thus the PSS state is equivalent to the (2, 2)-VBS state of spin-2 diagonal spin chain. The *non*-existence of the quantum phase transition in the in-phase dimerization case (left-upper in Fig. 1) is also well understood by the same procedure, i.e., in this whole region the ground state is in the (2, 2)-VBS phase for the diagonal composite S=2 spin. The interpretation of the ferromagnetic rung region (R < 0) is similar by making the S =2 composite spin from the two S=1 spins on a rung. On the line R = -1, which is equivalent to the spin-2 dimerized AF chain, there exists two critical points, and they are continued to the critical point of the spin-1 dimerized chain on the R = 0 line separating the (2,2)-, (3,1)-, and (4,0)-VBS states of the spin-2 composite rung spin chain. We have confirmed that each phase can be characterized by the spin-2 generalized string order parameters [7,9], and by the ground-state expectation value of the twist operator [6].

The above arguments on the spin-1 ladder is a natural generalization of that on the spin-1/2 non-dimerized ladder by Nishiyama $et\ al\ [10]$. By introducing bond alternation, the similar phase diagram to that of spin-1 ladder can be drawn. The generalization to the cases with larger S is straightforward.

To summarize, for the ground state of spin-S two-leg ladder the naive VBS picture breaks down. However, by making an appropriate composite spin-2S chain, we can identify each phase in spin-S ladder as that appears in spin-2S dimerized chain. The composite spin is made from the diagonal spins on the plaquette when the rung coupling is AF, and from the rung spins when the rung coupling is ferromagnetic.

References

- I. Affleck, T. Kennedy, E. H. Lieb, H. Tasaki, Phys. Rev. Lett. 59 (1987) 799.
- [2] M. den Nijs and K. Rommelse, Phys. Rev. B 40 (1989) 4709; H. Tasaki, Phys. Rev. Lett. 66 (1991) 798.
- [3] S. Todo, M. Matsumoto, C. Yasuda, H. Takayama, Phys. Rev. B 64 (2001) 224412.
- [4] M. Matsumoto, S. Todo, C. Yasuda, H. Takayama, Prog. Theor. Phys. Suppl. 145 (2002) 221.
- [5] S. Yamamoto, T. Sakai, A. Koga, J. Phys. Soc. Jpn. 71 (2002) 1250.
- [6] M. Nakamura, S. Todo, the 57th annual JPS meeting, 26pXY-8; M. Nakamura, S. Todo, Phys. Rev. Lett. 89 (2002) 077204.
- [7] M. Oshikawa, J. Phys.: Condens. Matter 4 (1992) 7469.
- [8] H. G. Evertz, unpublished (cond-mat/9707221); B. B. Beard, U.-J. Wiese, Phys. Rev. Lett. 77 (1996) 5130; S. Todo, K. Kato, Phys. Rev. Lett. 87 (2001) 047203.
- [9] S. Yamamoto, Phys. Rev. B 55 (1997) 3603

[10]Y. Nishiyama, N. Hatano, M. Suzuki, J. Phys. Soc. Jpn. ${\bf 64}~(1995)~1967.$